

## ADVANCED MATERIALS

### **Preparation and the study of the soft magnetic composites with ferrite as an insulation part.**

supervisor: doc. RNDr. Ján Fúzer, PhD. (jan.fuzer@upjs.sk)

study form: full time

Annotation: The study is oriented on the preparation and the investigation of the Fe based composite materials with ferrite as a nonconductive binder. Potential advantage of soft magnetic ferrites when used as electroinsulating layer instead of other insulations is their ferrimagnetic behavior, improving the magnetic interaction between the ferromagnetic powder particles in the final composite. Part of the work is the investigation of the electrical resistivity, wideband complex permeability and energy losses in prepared soft magnetic composites. The aim is optimization of preparation process (composition, method of preparation of hybrid powder material, pressing parameters, annealing parameters) of soft magnetic materials with required magnetic properties at middle-frequencies.

### **Study of magnetic and thermal properties of high-entropy functional alloys.**

supervisor: prof. RNDr. Rastislav Varga, DrSc. (rastislav.varga@upjs.sk)

consultant: Ing. RNDr. Andrea Džubinská, PhD.

study form: full time

Annotation: The main idea of the dissertation thesis is to find a suitable chemical composition that will meet the criteria for high-entropic functional alloys. Appropriately chosen composition of individual chemical elements leads to the preparation of such materials, focusing on selected physical properties. We will focus on combining elements belonging to the group of half Heusler alloys with the stoichiometric formula XYZ, where X and Y represent a transition element and Z an element from the p block. The preparation of samples in the form of strips and microwires using the Taylor-Ulitovsky method seems very advantageous for the materials we want to deal with. Part of the work is also the design of possible cooling technology and its implementation in technical practice.

### **Study of Heusler alloys with selected transport properties.**

supervisor: prof. RNDr. Rastislav Varga, DrSc. (rastislav.varga@upjs.sk)

consultant: RNDr. Ladislav Galdun, PhD.

study form: full time

Annotation: Heusler alloys cover many intermetallic alloys, which exhibit different significant physical properties such as thermoelectricity, superconductivity, spin polarization, shape-memory effect, and many others. The most significant advantage of Heusler alloys lies in the ability to tune their physical properties using various attributes such as chemical composition, valence electron concentration, structure, and others. The mentioned work focuses on the preparation and characterization of Heusler alloys with selected transport properties and with regard to the application potential. The alloys will be prepared in various forms and subsequently analyzed by available physical

methods. The main goal of this work is to find key parameters in selected groups of Heusler alloys in order to optimize application possibilities.

### **Surface deformation of magnetic domain walls in thin wires.**

supervisor: RNDr. Kornel Richter, PhD. (kornel.richter@upjs.sk)

consultant: prof. RNDr. Rastislav Varga, DrSc.

study form: full time

Annotation: Cylindrical topography of ferromagnetic samples is one of the crucial factors that contributes to a high domain wall velocity. In our work, we will focus on time-resolved observation of a surface domain wall shape in thin wires. We will employ a novel experimental setup based on Magneto-optical Kerr effect (MOKE), that will be extended by an option to observe multiple domain walls simultaneously. Student will participate on design of excitation coils and simulations of magnetic fields. Observations of a surface domain wall deformation will be carried out on samples differing by magnetic anisotropies.

### **Modeling of structural and magnetic properties of nanocomposites.**

supervisor: doc. RNDr. Adriana Zeleňáková, PhD. (adriana.zelenakova@upjs.sk)

consultant: RNDr. Pavol Hrubovčák, PhD.

study form: full time

Annotation: Advanced methods of material preparation allow for production of complex nanoscale systems consisting of several different structures. Each of the structures possesses its specific function and when combined and joined into single system one can obtain unique and smart nanocomposites. Owing to their specific properties, as prepared multifunctional nanomaterials are currently employed in technical, but foremost in the biomedical applications (theranostics). The proposed work will be devoted to the group of nanoscale systems consisting of superparamagnetic nanoparticles, amorphous silica (SiO<sub>2</sub>) and other specific ligands. The major objective of the proposed topic will be the study of the complex nanoparticle systems by means of modeling of their structural and magnetic properties (Matlab, Octave). The models will be designed and tailored in order to fit the best to the series of experimental data (structural measurements, magnetometry). With the aid of proposed models, the phenomena experimentally observed in the particular nanoscale system will be described, explained and the values of crucial parameters extracted. The models will be designed obeying the principles of generality and flexibility allowing their facile modification and application to the series of materials of the similar kind.

### **Preparation and study of electro catalyst and photo electro catalyst for hydrogen production by water splitting.**

supervisor: Mgr. Vladimír Komanický, PhD. (vladimir.komanicky@upjs.sk)

study form: full time

Annotation: The transition to renewable energy sources is recognized as one of the greatest societal challenges of the 21st century, and it will have a major impact on climate, environment and economy. The major bottleneck for broader utilization of renewable energy is a missing largescale and long-term energy storage technologies

the last two decades, a lot of research effort was given to produce renewable hydrogen fuel from solar energy, because of the growing market for renewable hydrogen to be used in commercially-ready proton-exchange membrane (PEM) fuel cells in fork lifts or cars. We refer to recent economic analysis and remark that hydrogen storage is not anymore the largest challenge. The PEM fuel cell is almost an ideal electricity-producing device, whose output is only water vapor without CO<sub>2</sub> emissions. From the variety of approaches for solar hydrogen production, most relevant technologies include: i) the use of water electrolyzers with excess renewable energy and ii) the photoelectrochemical (PEC) hydrogen production. While the first approach is already commercial, challenges remain to make electrolyzers cheaper and long-term stable. The development is focused on discovery of new catalytic materials. Second approach requires also discovery of new catalyst photoactive materials. In this thesis new catalytic materials for traditional electrolyzers and photocatalyst for photoelectrochemical water splitting will be developed using various techniques including physical deposition techniques. Activity and stability of catalysts will be tested using standard electrochemical tools.

### **The study of dynamic magnetic properties and relaxation process in magnetic nanoparticles.**

supervisor: doc. RNDr. Adriana Zeleňáková, PhD. (adriana.zelenakova@upjs.sk)

study form: full time

Annotation: Mono-domain metal nanoparticles based on iron and cobalt are of great interest due to their intrinsic physical properties, such as macroscopic quantum tunnelling (MQT), quantum size effects, giant magnetic moment and surface spin frustration interplaying between the surface and core atoms. The spin structure of nanoparticles can be affected by inter-particle interactions. One of the powerful ways how to get a better insight into the nature of inter-particle interactions and estimate their strength is the analysis of ac magnetic susceptibility. The PhD. study is oriented on investigation of dynamic magnetic properties and analyses of relaxation processes. The aim is to study the possibility of change in relaxation processes by controlling the inter-particle interactions, energy barrier distribution, particles size, etc.

### **Structural study of disordered and quasi-ordered metallic alloys using electron and XRD scattering.**

supervisor: Ing. Vladimír Girman, PhD. (vladimir.girman@upjs.sk)

consultant: prof. RNDr. Pavol Sovák, CSc.

study form: full time

Annotation: Phase transitions of solids from the disordered state to complex structures ordering are subject of modern research. The relationship between initial and final structure state play an important role at forming of the new structures having advanced physical and chemical properties. The variations of external conditions, e.g. strong magnetic fields or extremal temperature changes, can substantially affect the final properties of solids as well. The main highlight of dissertation thesis will be the study of atomic structure and stability of induced phases of promising advanced materials in relation to their properties, employing electron and X-ray diffraction techniques. The experimental approach, using transmission electron microscope JEOL 2100F UHR, will be emphasized. However, for successful completing of dissertation thesis, it will be

necessary to carry out experiments at electron microscopy centres and synchrotron facility abroad.

## **Institute of Experimental Physics SAS Košice**

### **Study of the atomic structure of materials with a high degree of disorder.**

supervisor: RNDr. Jozef Bednarčík, PhD. (bednarcik@saske.sk)

study form: full time

Annotation: Metallic glasses and nanocrystalline materials prepared by their heat treatment have a number of interesting mechanical and magnetic properties. Their excellent properties have originate in their unique atomic structure, which is characterized by a short-range atomic arrangement. X-ray scattering is an effective methodology for qualitative and quantitative description of atomic structure. At the same time, it allows to identify correlations between selected properties and corresponding changes in their structure. Nowadays, methods for modeling the atomic structure of amorphous substances using Monte Carlo-type simulation techniques are becoming increasingly popular. Within the proposed topic, attention will be paid to the identification of correlations between selected properties (magnetic and / or mechanical) and structural characteristics of the studied materials, having a high degree of internal atomic disorder. One of the main goals will be to model their atomic structure using the Monte Carlo method, using experimental data obtained by scattering of high-energy photons.

### **Study of the structure and superconducting properties of LREBCO bulk superconductors.**

supervisor: Ing. Pavel Diko, DrSc. (dikos@saske.sk)

consultant: Mgr. Vitaliy Antal, PhD.

study form: full time

Annotation: REBa<sub>2</sub>Cu<sub>3</sub>O<sub>x</sub> (REBCO, RE: Y or rare earth) bulk single grain superconductors (BSS) based on light rare earth (LRE) show record values of trapped magnetic field (17.6 T at 26 K for GdBCO BSS platinum alloyed) at reduced brittleness due to addition of silver. Research is currently looking at systems in which the addition of platinum is replaced by cheaper elements. Within the proposed topic, attention will be paid to the preparation of bulk LREBCO single crystals with selected alloying elements, analysis of their microstructure and characterization of their local and macroscopic superconducting properties. The methods of structural and phase analysis by electron microscopy, EDS and EBSD analysis, X-ray diffraction analysis, thermal analysis, magnetization measurements, measurements of the trapped magnetic field and levitation force will be used.

### **Soft magnetic nanocrystalline alloys based on 3-d metals prepared by unconventional thermal processing techniques.**

supervisor: RNDr. Ivan Škorvánek, CSc. (skorvi@saske.sk)

consultant: Ing. Branislav Kunca, PhD.

study form: full time

Annotation: The PhD thesis is focused on the employment of unconventional techniques of thermal processing in order to tailor the structural and magnetic properties of nanocrystalline alloys based on 3-d metals. We plan to use facility for ultra-rapid annealing of thin metallic ribbons constructed recently at IEP SAS. In this facility, the annealed samples are clamped between pair of the pre-heated massive Cu-blocks and typical annealing times take few seconds. High heating rates and much shorter processing times as compared to conventional annealing allow extend the composition interval where the annealed samples are still capable to form nanocrystalline structure. The other technique of thermal processing in this work is the annealing in a presence of high magnetic fields (up to 14 T). We plan to perform a detailed study of the corresponding changes of structural and magnetic properties caused by application of the above mentioned thermal processing to selected alloy systems.

### **Multifunctional magnetic nanomaterials for use in medicine.**

supervisor: Ing. Vlasta Závíšová, PhD. (zavisova@saske.sk)

consultant: RNDr. Martina Kubovčíková, PhD.

study form: full time

Annotation: Most biological processes take place at the nanoscale, and this gives us the opportunity to understand these processes and create new materials thanks to technical progress. Magnetic nanomaterials have considerable potential for use in medicine, e.g. in the distribution of the drug to the affected areas, in imaging but also in therapy. The main goal of the dissertation is not only the preparation of new magnetic nanomaterials, the binding of biologically active substances and the study of their physicochemical properties such as size, shape, structure, surface charge, magnetic properties, but also the investigation of their suitability for use. in the field of magnetic resonance diagnostics and the treatment of diseases e.g. by magnetic hyperthermia.

## **Institute of Materials Research SAS, Košice**

### **Electrocatalysts for future electrolyzers.**

supervisor: RNDr. Magdaléna Strečková, PhD. (mstreckova@saske.sk)

study form: full time

Annotation: The development of activities in the field of hydrogen technologies was also supported by the European Commission in the strategic document "Hydrogen Strategy for a Climate Neutral Europe". Today, Slovakia has suggested own national hydrogen strategy. The Hydrogen Technology Center is being established in Košice with the main "Power-to-Gas" concept using renewable power energy sources. A significant source of hydrogen is water and the electrolysis of water is the most promising technology for hydrogen production. However, before it can be recognized as an economically significant resource for large scale application with an exceptional energy potential, the simple, efficient, and secure methods of hydrogen retrieval have to be developed. Intrinsic structures of TMP meet the criteria of outstanding electrocatalysts that could further improve their HER performance in membrane electrode assembly. Therefore, the main challenge of dissertation thesis (DT) will be devoted to reduce the production cost of HER and at the same time to maintain the high efficiency of polymer electrode water electrolysis.

Substantial aim of DT will be aimed to improve the PEM water electrolysis components mainly electrode materials based on modified carbon fibers electrocatalysts result in the technology which should be more approached to commercial markets.

### **Structure and properties of relaxor ferroelectrics.**

supervisor: RNDr. Vladimír Koval', PhD. (vkoval@saske.sk)

study form: full time

Annotation: The dissertation will be focused on the research and development of advanced electroceramics, derived from perovskite-structured relaxor ferroelectrics, for effective energy storage. In course of dissertation work, theoretical and experimental approaches will be employed including material processing, X-ray diffraction and the Rietveld refinement method, scanning and transmission electron microscopy, and characterization of specific electro-physical properties of functional ceramics. For analytical assessment of the macroscopic properties with respect to the chemical and structural nature of electroceramics, an extended technique of dielectric spectroscopy will be adopted to study ferroelectric phase transitions.

### **Modelling of phase diagrams and thermodynamic properties of the systems for high temperature applications.**

supervisor: RNDr. Viera Homolová, PhD. (vhomolová@saske.sk)

Annotation: The work will be focused on the study of phases, phase equilibria and phase diagrams in the systems for high-temperature applications. The aim is to refine the uncertainty of phase diagrams and investigate unknown parts of selected binary systems by experimental methods of differential thermal analysis, X-ray diffraction and electron microscopy and then to model their phase diagrams and thermodynamic properties using the semi-empirical Calphad-method. The subjects of the study are binary systems with iridium. Iridium is an element which, due to its thermodynamic properties, is very interesting for use in the aerospace industry and due to its high corrosion resistance even at very high temperatures, it may potentially be suitable for use as part of gas turbine materials. The results of the thesis will allow extending the possibility of designing new materials for high-temperature use by computational methods without the need for time-consuming experimental testing.

### **Highly ionized plasma sputtering of multicomponent high entropy ceramic coatings.**

Supervisor: doc. RNDr. František Lofaj, DrSc. (flofaj@saske.sk)

study form: full time

Annotation: The development of magnetron sputtering is oriented toward technologies with high ionization degree of the sputtered material which provides better control of the deposition process as well as better coating properties. The most famous ionized PVD is the High Power Impulse Magnetron Sputtering (HiPIMS) and the relatively new technology High Target Utilization Sputtering (HiTUS) also belongs among these methods. High degree of ionization is achieved in the case of HiPIMS by very short duty cycle impulses with extremely high power density whereas in HiTUS by the power at an independent plasma source. The work should focus on the optimization of the deposition parameters of hard

multicomponent carbide, boride and nitride coatings from the viewpoint of the control of their elastic and plastic properties by means of determination of dependencies among the deposition parameters, plasma characteristics, coating structures and their mechanical and tribological properties. The work will be performed on the iPVD systems Cryofox Discovery (Polyteknik, Denmark) and HiTUS C500 (PQL, UK) in combination with the electron microscopy observations (SEM, TEM) and measurements of mechanical properties.

### **Quantitative characterization of plasma deposition of ceramic coatings by optical and electron spectroscopy methods.**

supervisor: doc. RNDr. František Lofaj, DrSc. (flofaj@saske.sk)

study form: full time

Annotation: The advanced ceramic coatings for ultrahigh temperature applications consist of high melting point and heavy (Zr, Hf, Ru, W..) metallic elements strongly bonded with light elements (boron, nitrogen, oxygen, carbon with hydrogen) which result in difficulties in quantitative analysis when using conventional chemical methods. Usually, a combination of several analytical methods is necessary to obtain quantitative characterization of both light and heavy elements at the same time in the resulting compounds. However, the control of the coating composition requires also the control of the plasma composition during the deposition. Thus, the in situ methods of plasma composition should be combined with the methods applied to the coatings to determine the relationships controlling their chemistry, structure and properties. The work should employ both in-situ optical emission spectroscopy for the plasma control with the ex-situ glow discharge optical emission spectroscopy (GDOES), Raman spectroscopy as well as energy and wavelength disperse electron spectroscopy (and potentially also X-ray Photoelectron Spectroscopy (XPS) and Secondary Ion Mass Spectroscopy (SIMS)) methods on the carbide and boride based coatings for quantification of their chemistry to establish the correlations between the plasma characteristics and their structure and properties. The plasma study will be performed on the existing iPVD systems using OES system (Avantes, The Netherlands) and Raman microscope GDOES as well as on the EDS and WDS attached to the scanning electron microscopes. The introduction of new XPS and SIMS facilities is also anticipated..

### **Mathematical modelling of the processes during nanoindentation, scratch testing and tribological tests in composite systems using FEM.**

supervisor: doc. RNDr. František Lofaj, DrSc. (flofaj@saske.sk)

study form: full time

Annotation: The work is focused on a detail study of the processes of stress and deformation states during instrumented nanoindentation, scratch and tribological tests in the coated composite systems using finite element modelling (FEM) extended FEM (xFEM) and Cohesive Zone Model (CZM) methods and subsequent experimental verification. The work will be performed on thin coatings on substrates with different mechanical properties. The aim is to understand the details of damage mechanisms in coatings in dependence on the loading conditions as well as the optimization of the conditions for the measurement of the mechanical properties and tribological properties of the studied coatings.

